Phase transitions in two dimensions: From the hard-disk model to active systems

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The hard-disk model has exerted outstanding influence on computational physics and statistical mechanics. Decades ago, hard disks were the first system to be studied by reversible Markov-chain Monte Carlo methods satisfying the detailed-balance condition and by molecular dynamics. It was in hard disks, through numerical simulations, that a two-dimensional melting transition was first seen to occur even though homogeneous short-range interacting particle systems cannot develop crystalline order. Analysis of the system was made difficult by the absence of powerful simulation methods.

In recent years, we have developed a class of irreversible event-chain Monte Carlo algorithms that violate detailed balance. They realize thermodynamic equilibrium as a steady state with non-vanishing probability flows. A new factorized Metropolis filter turns them into a paradigm for general Monte Carlo calculations. I will show how the resulting Monte Carlo algorithm has allowed us to demonstrate that hard disks melt with a first-order transition from the liquid to the hexatic and a continuous transition from the hexatic to the solid. Analogous computations have also lead to our new understanding of two-dimensional melting for soft disks, that has been intensely studied in experiment.

Finally, I will discuss two-dimensional melting on a substrate (as it is realized in skyrmion systems), and for active particles, and will present a very recent application of the event-chain algorithm to Coulomb-type long-range-interacting systems.